Numerical Weather Prediction

Improvements in Ozone Data Assimilation at the Met Office

Forecasting Research Technical Report No. 454

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Abstract

In this paper, further developments of the Met Office ozone assimilation system are described.

In the first part of the paper, the assimilation of ozone data from the Solar Backscatter Ultraviolet radiometer (SBUV) is investigated. This work is an extension of the original Met Office ozone assimilation system, in which data from the High Resolution Infrared Sounder (HIRS) were assimilated. Initial trials with Old Dynamics and comparison with GOME data showed that including SBUV data often improved the ozone analyses, chiefly in the northern hemisphere where more SBUV data were available. Comparison with HALOE profiles showed a positive benefit from SBUV in the 50-5 hPa layer. The trials also showed that SBUV data did not improve the ozone analyses near the tropopause. This may be due to the poor vertical resolution of the SBUV data compared to HIRS channel 9 data in this region.

When the system was upgraded to run with New Dynamics an immediate difference was a degradation in the ozone initial conditions which was probably caused by the Old Dynamics to New Dynamics reconfiguration. However, the reduction of errors compared to GOME occurred more rapidly with time for the New Dynamics trial than for the Old Dynamics trial, suggesting that the HIRS channel 9 and SBUV data were being properly assimilated and that the poor initial conditions gradually get spun out of the system.

The second part of the paper describes further sensitivity tests and also the impact of including a parametrization of stratospheric ozone chemistry in the forecast model.

First, a criterion for rejecting HIRS channel 9 data in the observation processing system was made less stringent, and the impact of this was to reduce ozone analysis errors near the tropopause. Second, increasing the ozone background error covariance above the 20 hPa level generally led to reductions of 5-10 % in ozone analysis errors. Third, using analysed ozone in the UM radiation code (instead of a model climatology) reduces temperature analysis and forecast errors in the lower stratosphere.

Addition of a parametrization of stratospheric ozone chemistry, the so-called 'Cariolle scheme' greatly improves the ozone background field. Improvements to this background field when HIRS channel 9 and SBUV data are added to the assimilation are still seen, but they are smaller than in the corresponding pair of experiments in which the Cariolle scheme is not included.

1 Introduction

There are a number of reasons why adding ozone to the Met Office's 3D-Var assimilation scheme (Lorenc et al, 2000) could have a positive impact on numerical weather prediction (NWP). These include improved assimilation of satellite radiances, improved radiative heating, and improved predictions of UV radiation. Furthermore, the upgrading of the operational assimilation system to 4D-Var could allow scope for assimilated ozone to have a positive impact on wind fields through correlations between ozone and potential vorticity and other dynamic variables.

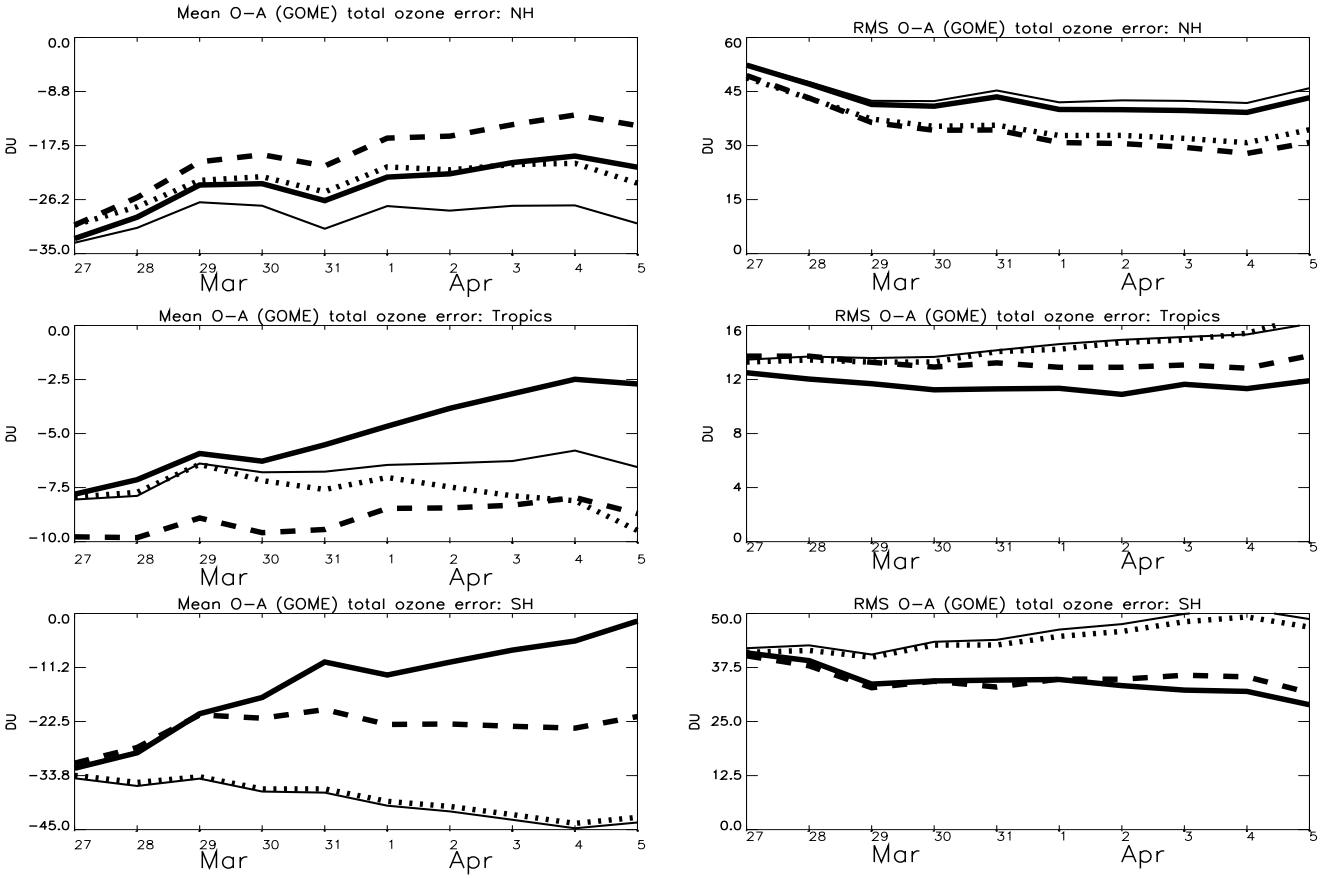

Figure 1: GOME total ozone minus analysed total ozone (DU), plotted against time, from 27/03/01-05/04/01. Mean (left panels) and RMS (right panels) for the northern hemisphere (30-90^{o}N) (top panels), tropics (30^{o}N-30^{o}S) (middle panels) and southern hemisphere (30-90^{o}S) (bottom panels). Analyses are run using Old Dynamics: control run (no ozone data assimilated) (thin solid line); HIRS channel 9 data assimilated (solid line); SBUV data (dotted line); HIRS channel 9 plus SBUV data assimilated (dashed line).

Jackson and Saunders (2002) described a preliminary ozone assimilation system in which data from the High Resolution Infrared Sounder (HIRS) were assimilated. Results were encouraging, and indeed the system formed the basis of a study to investigate the potential benefits of stratospheric ozone and wind observations from the planned Stratospheric Wind Interferometer For Transport studies (SWIFT) satellite instrument (Lahoz et al, 2003, 2004).

There is an abundance of ozone data available daily in near real time. In addition to HIRS data, global total ozone fields are available both from the Total Ozone Mapping Spectrometer (TOMS) and the Global Ozone Monitoring Experiment (GOME), and stratospheric ozone profiles can be inferred from Solar Backscatter

Ultraviolet radiometer (SBUV) observations. Therefore, it makes sense to extend the ozone assimilation system to include more of these datasets.

In the first part of this paper, I describe the the inclusion of SBUV data in the existing ozone assimilation scheme and the impact of these data on the ozone analyses. Section 2 contains details of the SBUV observation data processing, and of the SBUV forward model and adjoint used in 3D-Var. In Section 3 results of 10 day assimilation trials with SBUV assimilation appear.

Jackson and Saunders (2002) also described ways (other than the addition of SBUV data) by which the ozone assimilation system could be extended and improved. These included a new representation of background error covariances and the inclusion of the interaction between analysed ozone and the Unified Model (UM) radiation scheme. Morcrette (2003) investigated such an interaction in the ECMWF data assimilation system and concluded that the interaction had a positive impact on temperature forecasts between 100 and 10 hPa. Tests investigating these changes are described in Section 4.

Also of importance is the proper representation of ozone photochemistry. I have implemented the Cariolle scheme (Cariolle and Deque, 1986) to parametrize photochemical sources and sinks of ozone and the 'cold tracer' scheme (Hadjinicolaou et al, 1997) to represent ozone destruction due to heterogeneous chemistry. Tests of these schemes using forecast-only simulations and data assimilation trials are detailed in Section 5. Recommendations for future research appear in Section 6 and a Summary appears in Section 7.

2 Assimilation of SBUV Data

Ozone is included in the Met Office's 3D-Var assimilation scheme (Lorenc et al, 2000), and, for the initial experiments, the forecast model used is a 40 level version of the UM, with an Eulerian dynamical core ('Old Dynamics') and a top level near 0.1 hPa. Following upgrades to the forecast model, subsequent experiments used a 50 level version of the UM, with a semi-Lagrangian dynamical core ('New Dynamics') and a top level near 63 km. Both UM versions have a horizontal resolution of 2.5^o latitude x 3.75^o longitude. The background ozone field required for the assimilation is calculated using a tracer transport equation within the UM. Currently, the model radiation scheme uses climatological ozone rather than assimilated ozone. However, in Section 4.3 the interaction between assimilated ozone and radiative heating is investigated. The parametrization of the chemical production and loss of stratospheric ozone (following Cariolle and Deque, 1986) is omitted in most of the tests described here, apart from those described in Section 5.

Sections 2.1 and 2.2 describe in detail the quality control and assimilation of the SBUV data.

2.1 Quality Control of SBUV Data in the Observation Processing System (OPS)

The SBUV instrument flies on NOAA satellites and the processed ozone data is available in 12 layers. However, the profile information information above 1 hPa and below 16 hPa is determined mainly by climatology. Therefore, at ECMWF they have combined the layers to avoid correlated data, resulting in the following 6 layers: 0.1-1 hPa, 1-2 hPa, 2-4 hPa, 4-8 hPa, 8-16 hPa and 16 hPa to surface. The reprocessed data from ECMWF are ingested into the MetDB.

The major part of the quality control done in OPS is the background check, where data are accepted or rejected on the basis of a comparison with observation equivalents calculated from model background data.

The model equivalent of SBUV ozone observations are calculated from background ozone profiles. Let p_{oL} and p_{oU} be the lower and upper pressures of each SBUV layer, and assume that there are N model layers between these pressures, denoted by the indices j, j+1,...,j+N-1. Then the pressure weighted model ozone, O, in the SBUV layer is

$$O = O_{LB} + O_{MID} + O_{UB} \tag{1}$$

O_{MID} is the pressure weighted ozone between the model layers j and j+N-1, and is given by

$$O_{MID} = 1/2 \sum_{k=j}^{j+N-2} [(o_{3_k} + o_{3_{k+1}})(p_{m_k} - p_{m_{k+1}})] \quad (2)$$

where o_{3_k} is the background ozone mixing ratio at model level k, and p_{m_k} is the model pressure at level k.

O_{LB} and O_{UB} are the pressure weighted ozone amounts between p_{oL} and p_{m_j} and $p_{m_{j+N-1}}$ and p_{oU}, respectively.

$$O_{LB} = [[[(p_{m_{j-1}} - p_{oL})o_{3_j} + (p_{oL} - p_{m_j})o_{3_{j-1}}]/(p_{m_{j-1}} - p_{m_j})] + o_{3_j}](p_{oL} - p_{m_j}) \quad (3)$$

and

$$O_{UB} = [[[(p_{m_{j+N-1}} - p_{oU})o_{3_{j+N}} + (p_{oU} - p_{m_{j+N}})o_{3_{j+N-1}}]/(p_{m_{j+N-1}} - p_{m_{j+N}})] + o_{3_{j+N-1}}](p_{m_{j+N-1}} - p_{oU}) \quad (4)$$

The SBUV retrievals are in units of ozone density (kg m^{-2}). The conversion of pressure weighted ozone to ozone density, O_{den} is done by

$$O_{den} = O/g \quad (5)$$

where g = acceleration due to gravity.

Before performing the background check three other quantities need to be specified: observation error, background error and the probability density of bad observations. The observation error is also supplied by ECMWF. For simplicity it is assumed that the background error is three times the observation error, and the probability density of bad observations is assumed to be 0.01 $(kg/m^{-2})^{-1}$. Note also that these background errors are only used in the OPS quality control; different error covariances (derived from ECMWF analyses) are used in 3D-Var.

Following the background check, observations with a solar elevation less than 6^o or with a quality flag (provided by ECMWF) of greater than zero are blacklisted. The blacklist follows the approach used by ECMWF for their operational ozone analyses (A. Dethof, pers. comm.).

2.2 SBUV in 3D-Var

In order to assimilate SBUV data in 3D-Var, an observation operator and its adjoint need to be written. The approach of Ross Bannister (DARC) is followed and his contribution is acknowledged. Full documentation appears at
http://www.met.rdg.ac.uk/ ross/DARC/LayerAv.html,
and a summary appears below.

Forward Model The forward model calculation is similar to that shown in Section 2.2, except that the calculation of the O_{LB} and O_{UB} terms is slightly different. Here,

$$O_{LB} = [o_{3_{j-1}} + (dq/dp_{j-1})(p_{oL} - p_{m_{j-1}}) + o_{3_j}](p_{oL} - p_{m_j})/2 \tag{6}$$

and

$$O_{UB} = [2o_{3_{j+N}} + (dq/dp_{j+N})(p_{oU} - p_{m_{j+N}})](p_{m_{j+N}} - p_{oU})/2 \tag{7}$$

where

$$dq/dp_k = (o_{3_{k+1}} - o_{3_k})/(p_{m_{k+1}} - p_{m_k}) \tag{8}$$

If there are no model levels within the observation layer, equation (1) is replaced by

$$O = -[2o_{3_{j-1}} + (dq/dp_{j-1})(p_{oL} - 2p_{m_{j-1}} + p_{oU})](p_{oL} - p_{oU})/2 \tag{9}$$

Adjoint Model The equations for the adjoint are as follows.

For each observation layer i, and for each level, k, between j and j+N-1, the contribution to the gradient of the observation penalty with respect to ozone, $\delta\nabla_{q_k} J_o$, is

$$\delta\nabla_{q_k} J_o = f_k \nabla_{\hat{q}_i} J_o \tag{10}$$

$$\delta\nabla_{q_{k+1}} J_o = f_k \nabla_{\hat{q}_i} J_o \tag{11}$$

where $f_k = -(p_{m_{k+1}} - p_{m_k})/2g$, and $\nabla_{\hat{q}_i} j_o$ is the gradient of the observation penalty with respect to SBUV ozone density.

As with the forward model calculation, the contribution between between p_{oL} and p_{m_j} and $p_{m_{j+N}}$ and p_{oU}, respectively, also has to be added.

At the lower boundary, this is

$$\delta\nabla_{q_{j-1}} J_o = (f_1 - f_3)\nabla_{\hat{q}_i} J_o \tag{12}$$

$$\delta\nabla_{q_j} J_o = (f_1 + f_3)\nabla_{\hat{q}_i} J_o \tag{13}$$

where $f_1 = -(p_{m_j} - p_{oL})/2g$, $f_2 = (p_{oL} - p_{m_{j-1}})/(p_{m_j} - p_{m_{j-1}})$ and $f_3 = f_1\ f_2$.

and at the upper boundary, this is

$$\delta\nabla_{q_{j+N}} J_o = (2f_4 - f_6)\nabla_{\hat{q}_i} J_o \tag{14}$$

$$\delta\nabla_{q_{j+N+1}} J_o = f_6 \nabla_{\hat{q}_i} J_o \tag{15}$$

where $f_4 = -(p_{oU} - p_{m_{j+N}})/2g$, $f_5 = (p_{oU} - p_{m_{j+N}})/(p_{m_{j+N+1}} - p_{m_{j+N}})$ and $f_6 = f_4\ f_5$.

If there are no model levels within the observation layer, equations (10) and (11) are replaced by

$$\delta\nabla_{q_{j-1}} J_o = (p_{oL} - p_{oU})(1 - f_7)\nabla_{\hat{q}_i} J_o \tag{16}$$

$$\delta\nabla_{q_j} J_o = (p_{oL} - p_{oU}) f_7 \nabla_{\hat{q}_i} J_o \tag{17}$$

where $f_7 = -(p_{oU} + p_{oL} - 2p_{m_{j-1}})/(2g(p_{m_j} - p_{m_{j-1}}))$.

The terms of the left hand side of equations (10) - (17) are summed over all observation layers to produce the total gradient of the observation penalty with respect to ozone.

3 Trial Results

The data assimilation trials were run for 10 days starting from 12Z on 26th March 2001. All initial conditions were taken from the operational Met Office stratospheric analysis from that time, with the exception of the ozone field, which used March monthly mean values from the climatology of Li and Shine (1995).

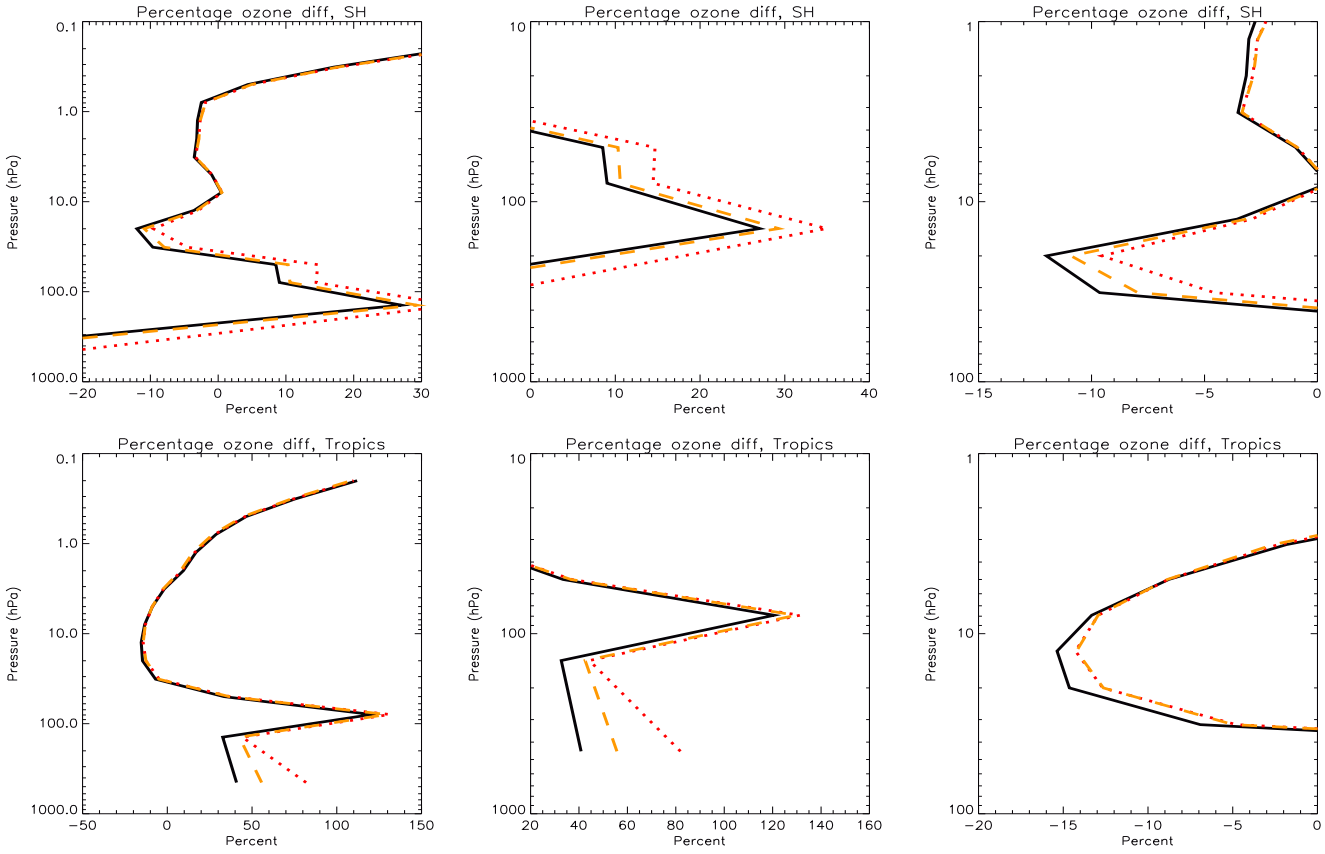

Figure 2: Percentage difference between HALOE and analysed ozone profiles (100 (O-A) / O, where O = HALOE ozone and A=analysed ozone), averaged over the trial period (27/03/01-05/04/01). Top panels show values for the southern hemisphere (30-90°S) and bottom panels show values for the tropics (30°N-30°S). Left panels are for the 100-0.1 hPa pressure range. Middle and right panels focus on the 1000-10 hPa and 100-1 hPa ranges, respectively. Analyses assimilate HIRS channel 9 (black solid line), SBUV (red dotted line) and HIRS channel 9 plus SBUV (orange dashed line).

3.1 Runs with Old Dynamics

The SBUV code was initially developed and tested using the Old Dynamics system. Comparisons were made with runs where the only ozone data assimilated was from HIRS channel 9 radiances to show the impact of SBUV on the analysed fields.

Figure 1 shows analysed total ozone compared with GOME total ozone for four experiments. In the control run, all available operational observations are assimilated, but ozone data (ie from HIRS channel 9 and SBUV) are not. Ozone is merely advected as a passive tracer in the UM.

When HIRS channel 9 radiances are added, there is a reduction in the bias and RMS error of the ozone analysis at all latitudes. The reduction is strongest in the southern hemisphere. This is because the HIRS data are only assimilated over the sea and in clear sky conditions, and since there is more sea in the southern

hemisphere, more HIRS data are used there than in other latitude zones. For a further discussion of the HIRS 9 results see Jackson and Saunders (2002).

When only SBUV data are used the only positive impact appears to be in the northern hemisphere. Furthermore, the northern hemisphere is the only zone where the errors in the run where both HIRS 9 and SBUV data are used are smaller than for those in the runs where HIRS 9 and SBUV data are used individually.

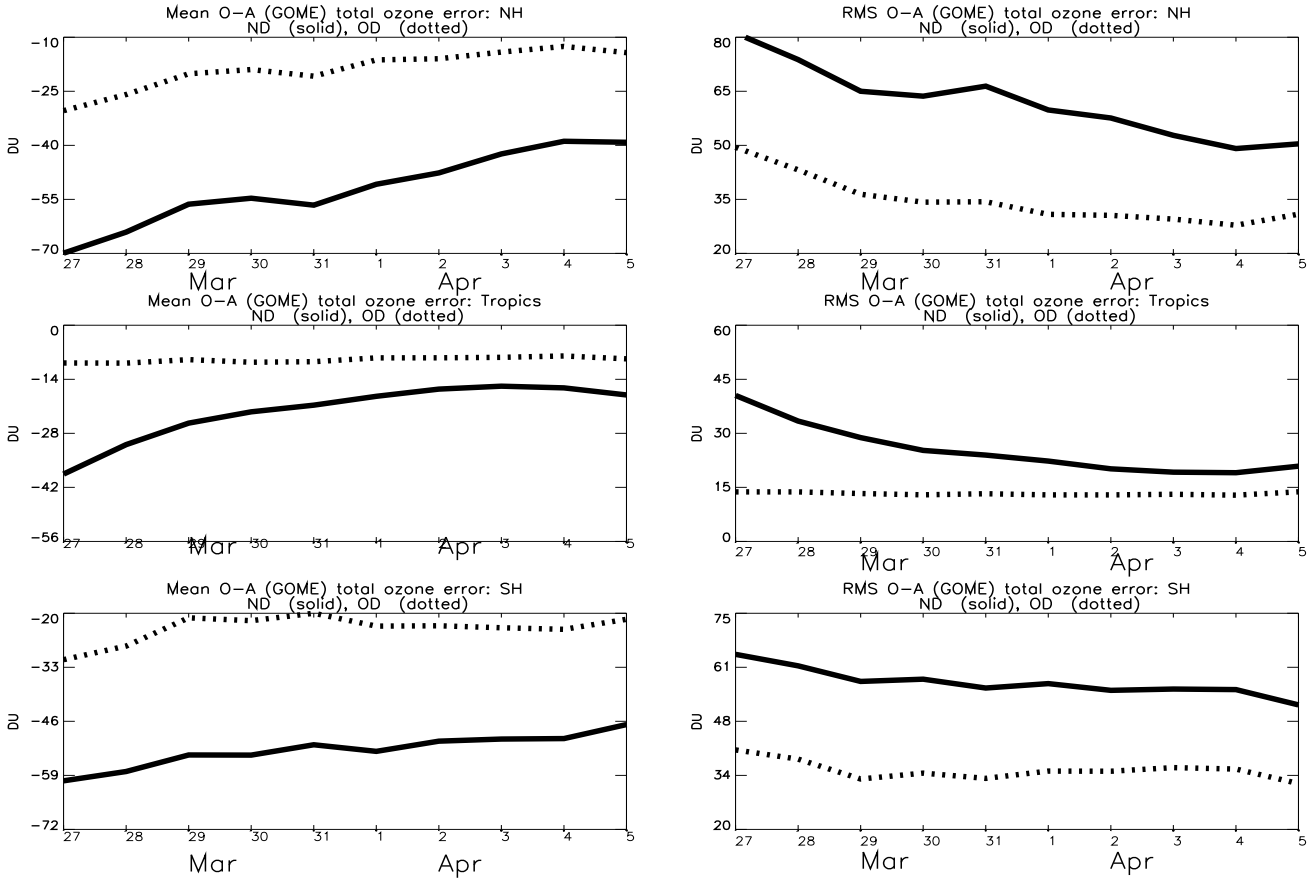

Figure 3: GOME total ozone minus analysed total ozone (DU), plotted against time, from 27/03/01-05/04/01. Mean (left panels) and RMS (right panels) for the northern hemisphere (30-90^{o}N) (top panels), tropics (30^{o}N-30^{o}S) (middle panels) and southern hemisphere (30-90^{o}S) (bottom panels). Analyses are run using Old Dynamics (dotted line) and New Dynamics (solid line).

The explanation for this is twofold. First, in the trial period there are far more SBUV observations in the northern hemisphere than at other latitudes and therefore one would expect their impact to be greatest there. Second, Figure 1 shows column ozone, which is not the best way of showing the impact of SBUV, which varies with height.

More revealing is to compare analysed ozone profiles with HALOE profiles (Figure 2). The Figure shows the percentage difference between HALOE and analysed profiles for the tropics and the southern hemisphere (unfortunately HALOE did not observe in the northern hemisphere during the trial period). The differences are shown for the 1000-0.1 hPa range, and also for the 1000-10 hPa and 100-1 hPa ranges, with different abscissa ranges for clarity. It is clear that introducing the SBUV data reduces the error with respect to HALOE in the stratosphere between around 50 and 5 hPa. However, the analysis around 100 hPa is poorer when SBUV data is introduced. This may be because the SBUV data at these levels cannot describe the vertical ozone structure as well as the HIRS channel 9 data. The SBUV data assimilated at these levels are simply layer averages from 1000 to 16 hPa, whereas the sensitivity of HIRS channel 9 to ozone (as expressed by the ozone Jacobian) has a peak centred in the upper troposphere, and is close to zero near the surface and above

the lower stratosphere.

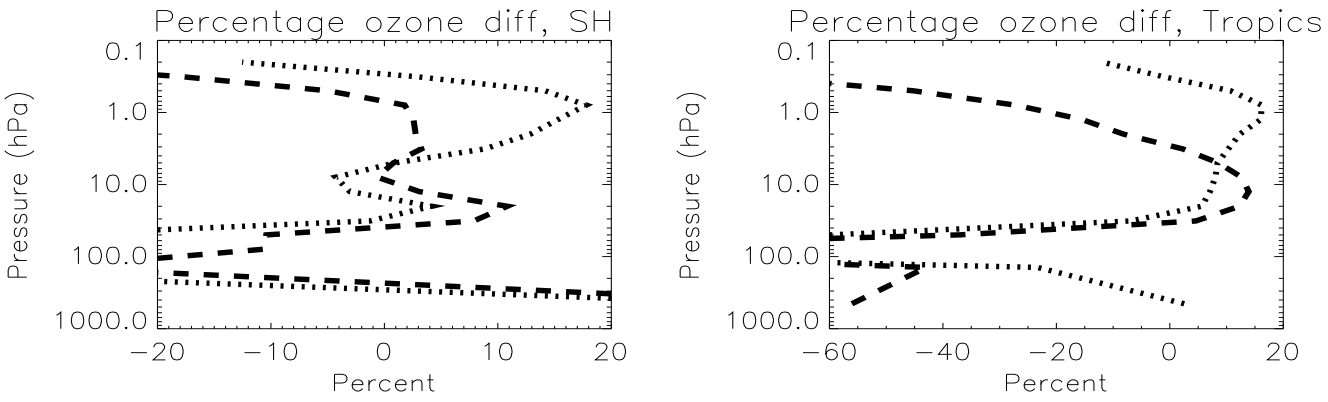

Figure 4: Percentage difference between HALOE and analysed ozone profiles (100 (O-A) / O, where O = HALOE ozone and A=analysed ozone), averaged over the trial period (27/03/01-05/04/01). The left panel shows values for the southern hemisphere (30-90^{o}S) and the right panel shows values for the tropics (30^{o}N-30^{o}S), for analyses run using Old Dynamics (dashed line) and New Dynamics (dotted line).

The latter result suggests that it may be a good idea to omit SBUV data from the 1000-16 hPa layer from the assimilation. Note, however, that these results must be treated with some caution, because of the poor quality of HALOE data near the tropopause (Bruhl et al, 1996) and the low numbers of SBUV observations available in the tropics and southern hemisphere during the trial period.

3.2 Runs with New Dynamics

Having achieved acceptable results with SBUV data run with Old Dynamics, the next imperative was to upgrade the system to run with New Dynamics. This involved alteration of the OPS and VAR code and proved to be rather time-consuming.

Figure 3 shows a comparison of Old Dynamics and New Dynamics results for experiments in which both HIRS channel 9 and SBUV data were assimilated. The clearest difference between the results is that, initially, the negative bias in O-A is larger for the New Dynamics run and the RMS error is also larger. The reason for this difference is that the reconfiguration required to create a New Dynamics start dump from an Old Dynamics start dump lowers the peak in the stratospheric ozone field, and thus the initial conditions are even further away from the GOME correlative measurements.

Despite the differences in the initial fields, Figure 3 shows that the New Dynamics analyses move closer to the GOME analyses with time, and they do so at a faster rate than the Old Dynamics analyses, suggesting that the poor initial conditions are gradually getting spun out of the system.

Figure 4 compares the Old Dynamics and New Dynamics analysed ozone profiles with HALOE data. This also shows the impact of the different initial conditions, with the O-A differences for the New Dynamics run being more positive in the upper stratosphere and more negative in the lower and middle stratosphere.

Subsequent to these trials, a bug was discovered in the SBUV adjoint code which meant that ozone increments from the uppermost SBUV layers were not being added correctly. This bug was fixed and the trial re-run. The impact of this change on the analysed total ozone field is small, since it affects levels where the pressure is small. It can be seen more clearly by comparing ozone profiles, such as in Figure 5. This Figure shows that the bug fix reduces the difference between analysed and HALOE ozone at most levels above 10 hPa.

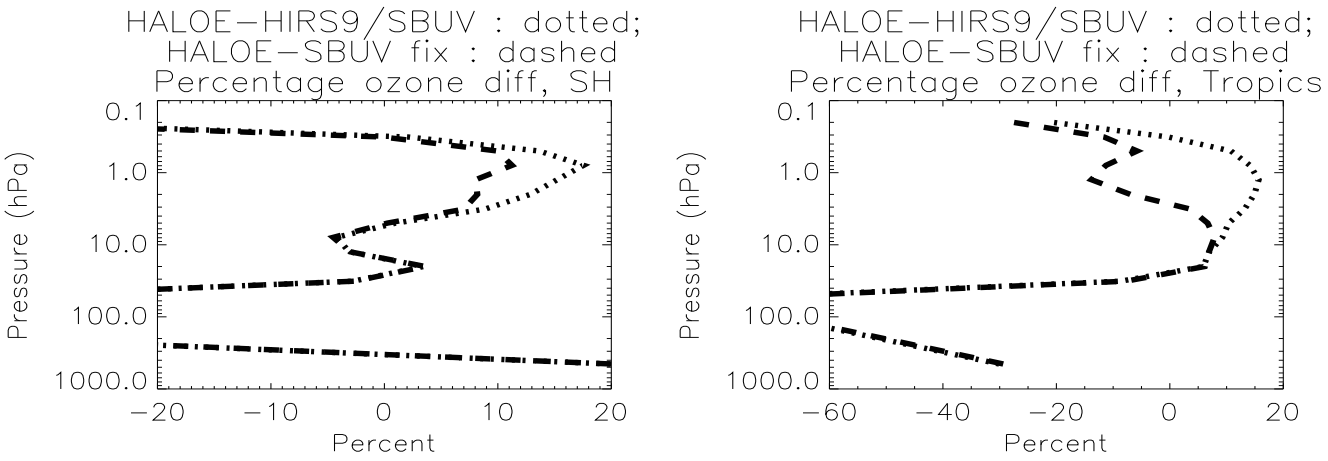

Figure 5: Like Figure 4, except data for the original New Dynamics HIRS channel 9 / SBUV run (dotted line) and the re-run with the SBUV adjoint bug fixed (dashed line) are shown.

4 Other Sensitivity Runs

4.1 A Less Stringent Criterion for Rejecting HIRS Channel 9 data

The initial tests of the ozone assimilation assimilation scheme using New Dynamics were run on the T3E using a version of OPS (Stable12.1) which still used separate Extract and Process steps. Figure 6 shows a comparison of such results for runs with and without the ozone assimilation switched on. We can infer quite a lot about the relative impacts of HIRS channel 9 and SBUV data on the analysis without having to run separate experiments. This is because more SBUV data are available in the northern hemisphere than in other locations, more HIRS channel 9 data are used in the southern hemisphere than in the northern hemisphere, and because the impact of the HIRS channel 9 data should be extremely small above the lower stratosphere, because its ozone Jacobian is close to zero there.

The absolute difference plot (middle panel) largely shows the impact of the SBUV data on the ozone analysis. Since the HIRS channel 9 data mainly have an impact in the troposphere, where the ozone amounts are much lower than in the stratosphere, the impact of these data on the ozone analysis is better shown by looking at the relative difference between the two runs (right panel). The plots show that the SBUV data have the smallest impact in the southern hemisphere (where there are hardly any SBUV observations during the trial period) and that the impact of the HIRS channel 9 is largest in the southern hemisphere, where there is more sea and thus where fewer data are rejected in the OPS.

When the code was transferred to the SX6 it was also upgraded to OPS/VAR Stable 20.1. This version includes the new combined Extract and Process step in OPS. Figure 7 is like Figure 6, except that the SX6/Stable 20.1 results are shown. The impact of the SBUV observations is similar to before but the impact of the HIRS channel 9 data is much smaller. On further examination it was found that far more HIRS channel 9 data were rejected in OPS with Stable 20.1 than with Stable 12.1.

A large number of these extra rejected data were thrown out because they failed the check of retrieved brightness temperatures against expected error. It is not clear why this difference has been introduced but presumably it is related to the switch to the combined Extract and Process step. A trial was run in which the rejection limit for retrieved minus observed brightness temperatures for HIRS channel 9 was increased by

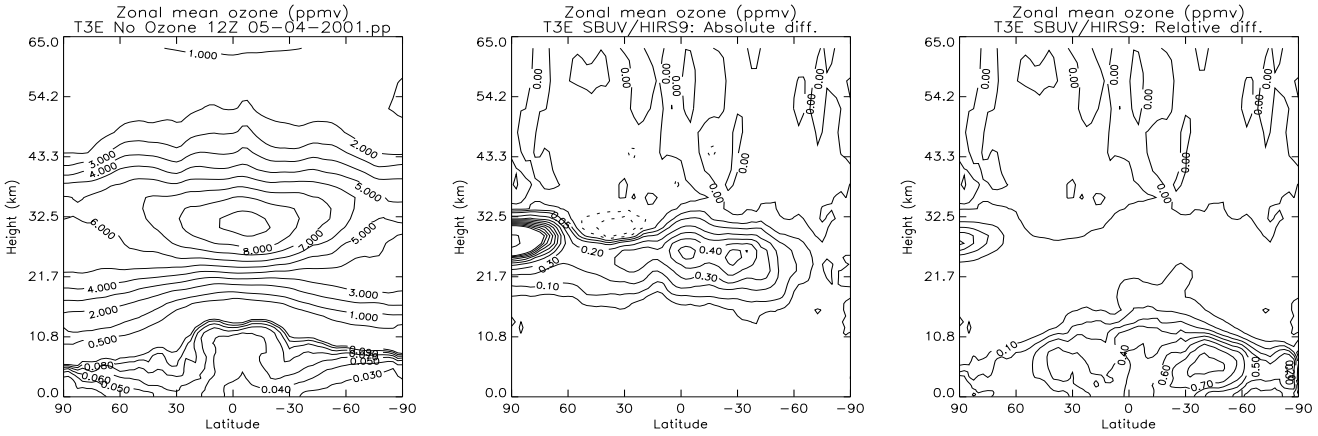

Figure 6: Zonal mean ozone for 05/04/01 for a run with no ozone assimilation (left panel), absolute difference between this run and a run which assimilated SBUV and HIRS channel 9 data (centre panel), and the relative difference between these two runs (right panel). Both runs were performed on the T3E using OPS Stable 12.1. Contours: ppmv

a factor of three. The results are shown in Figure 8. One can see that the impact of HIRS channel 9 data on tropospheric ozone is much larger than in Figure 7 and similar to that in Figure 6.

The impact of this change can also be seen in comparisons of these analyses with sonde data. Figure 9 shows percentage differences between ozonesonde profiles and analysed profiles. The effect of accepting more HIRS channel 9 data into the retrieval is that the analysis now better agrees with the sonde data, especially in the extratropics near the tropopause.

This change to the retrieved brightness temperature check is clearly beneficial to the ozone analysis and the relevant code has been lodged.

4.2 Impact of ozone background error covariances

A further trial was carried out to test the sensitivity of the assimilation to a change in the ozone background error covariances. It is believed that the variances used (which are supplied by ECMWF) may be too small in the middle and upper stratosphere and thus the model may be too strongly constrained to the background. Accordingly, the covariance matrix was altered so that the standard deviation between around 20 hPa and the model top was increased to be 10 % of a typical global mean climatological profile (see Lahoz et al (2003) for further details). The impact of this changes was generally positive, with reductions of 5-10 % seen in errors with respect to HALOE data. Whilst this is an encouraging result, future research will focus on a more comprehensive upgrade of ozone background errors, perhaps involving the derivation of statistics using the NMC method (Parrish and Derber, 1992), or from 6 hour differences from longer period runs (Y.J Rochon et al, pers. comm.).

4.3 Interaction between analysed ozone and radiative heating

A proposed benefit of ozone assimilation is that if the analysed ozone is used in the forecast model radiation scheme, then the radiative heating rates should be more accurate than when climatological ozone is used (as is the case at the Met Office and most other operational centres), and the forecast should benefit as a result. Morcrette (2003) investigated this interaction between ozone analyses and radiative heating rates using the

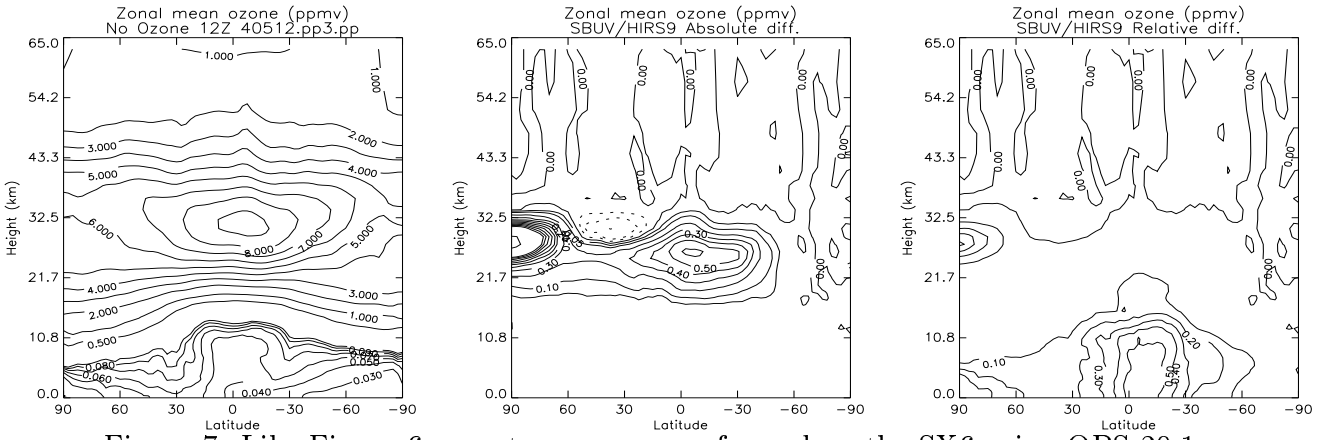

Figure 7: Like Figure 6 except runs were performed on the SX6 using OPS 20.1

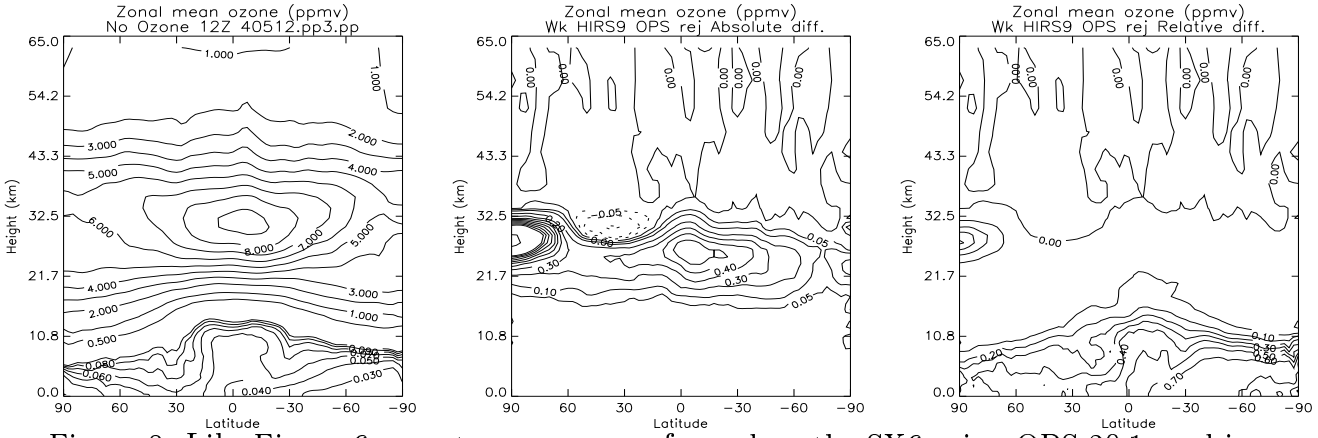

Figure 8: Like Figure 6 except runs were performed on the SX6 using OPS 20.1, and in the test run the rejection limit for retrieved minus observed brightness temperatures for HIRS channel 9 was increased by a factor of three.

ECMWF model. He compared 10-day forecasts made with and without ozone-radiation interactions. These interactions lead to a relatively small and generally positive impact on temperature forecasts between 100 and 10 hPa.

The impact of this ozone-radiation interaction in the Met Office system was investigated by running another 10 day trial for March / April 2001 with this interaction included. The impact on ozone and temperature analysis errors is very small, but temperature forecast errors are clearly reduced in the lower stratosphere, and this reduction is generally greater the longer the forecast time is (in these trials forecasts were run out to 72 hours). These impacts are illustrated in Figure 10, which shows mean and rms temperature errors, verified against sonde data, for 48 hour forecasts run with and without the ozone-radiation interaction. In all three latitude zones, the errors are reduced between 150 or 100 and 30 hPa when the ozone-radiation interaction is included, with the largest reduction generally in the 70-50 hPa layer. Above 30 hPa, the errors are reduced in the southern hemisphere and increase at other latitudes. The impact on temperature errors in the troposphere is generally very small.

The changes in the temperature errors can be better understood by looking at Figure 11. The fields shown here are valid for only one time, rather than being a time average, and thus of course the differences between them may be due to dynamical variability as well as to changes in radiative heating. The top panels show the 48 hour forecast ozone field for the run with the ozone-radiation interaction included, the climatological ozone field for the same time (which is used in the radiation scheme when no ozone-radiation interaction is included), and their difference. The former field is larger above 30 km (around 10 hPa) everywhere except in

the southern high latitudes. At such altitudes solar heating from ozone absorption greatly exceeds long wave cooling from ozone and so changes in the temperature field will be of the same sign as the ozone changes. This is generally seen in Figure 11 (bottom right panel) down to around 2 hPa (around 45 km). Temperature differences at the uppermost levels exceed 10 K. At and just below these levels, the temperature change is of the opposite sign, because the increased (decreased) ozone aloft allows fewer (more) photons to reach these levels, and the heating rate is thus less (greater). In the lowermost stratosphere the primary radiative impact of ozone is long wave heating, which is strongest in the tropics (eg Andrews et al (1987), Fig. 2.31, 2.32). Consistent with this, Figure 11 shows a correlation between ozone and temperature differences. Note, though, that the temperature differences do not exceed 0.3 K. Temperature differences in the troposphere are even smaller, often being less 0.1 K.

These results are encouraging and these experiments should be extended to include longer-period assimilation trials, or multi-annual climate simulations. The only correlative measurements currently used to validate the temperature forecasts are from sondes, but these are not available above the 10 hPa level. Given that the largest temperature changes are seen above this level, the results should be compared to other types of correlative data that are available at such altitudes, such as HALOE profiles.

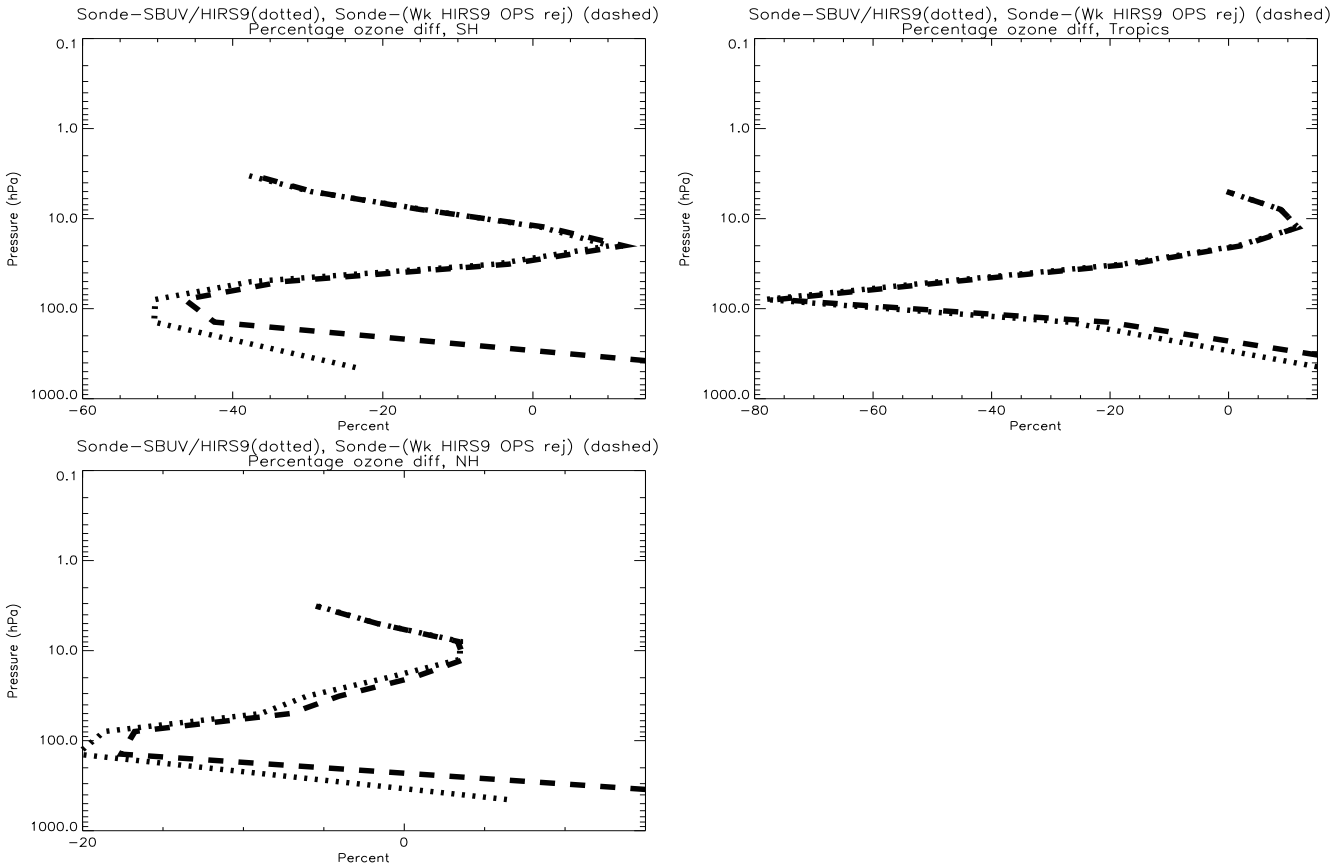

Figure 9: Percentage difference between ozonesonde and analysed ozone profiles (100 (O-A) / O, where O = sonde ozone and A=analysed ozone), averaged over the trial period (27/03/01-05/04/01). Profiles are shown for the southern hemisphere (30-90^{o}S), the the tropics (30^{o}N-30^{o}S) and the northern hemisphere (30-90^{o}N) for an initial SBUV / HIRS channel 9 assimilation (dotted line) and an assimilation in which the rejection limit for retrieved minus observed brightness temperatures for HIRS channel 9 was increased by a factor of three (dashed line).

5 Parametrization of Ozone Chemistry

The chemical production and loss of ozone plays a major role in determining the stratospheric ozone distribution. Thus, the background estimate of ozone can be greatly improved by including a parametrization of ozone chemistry in the UM. The Cariolle scheme (Cariolle and Deque, 1986) provides an efficient and reasonably realistic way of parametrizing the photochemical sources and sinks of ozone. It does this by approximating the net ozone photochemical production / loss rate as a function of three variables: the local ozone mixing ratio, temperature and the overlying ozone column abundance. In addition, the so-called 'cold tracer' scheme (Hadjinicolaou et al, 1997) represents ozone destruction due to heterogeneous chemistry associated with Polar Stratospheric Clouds (PSCs).

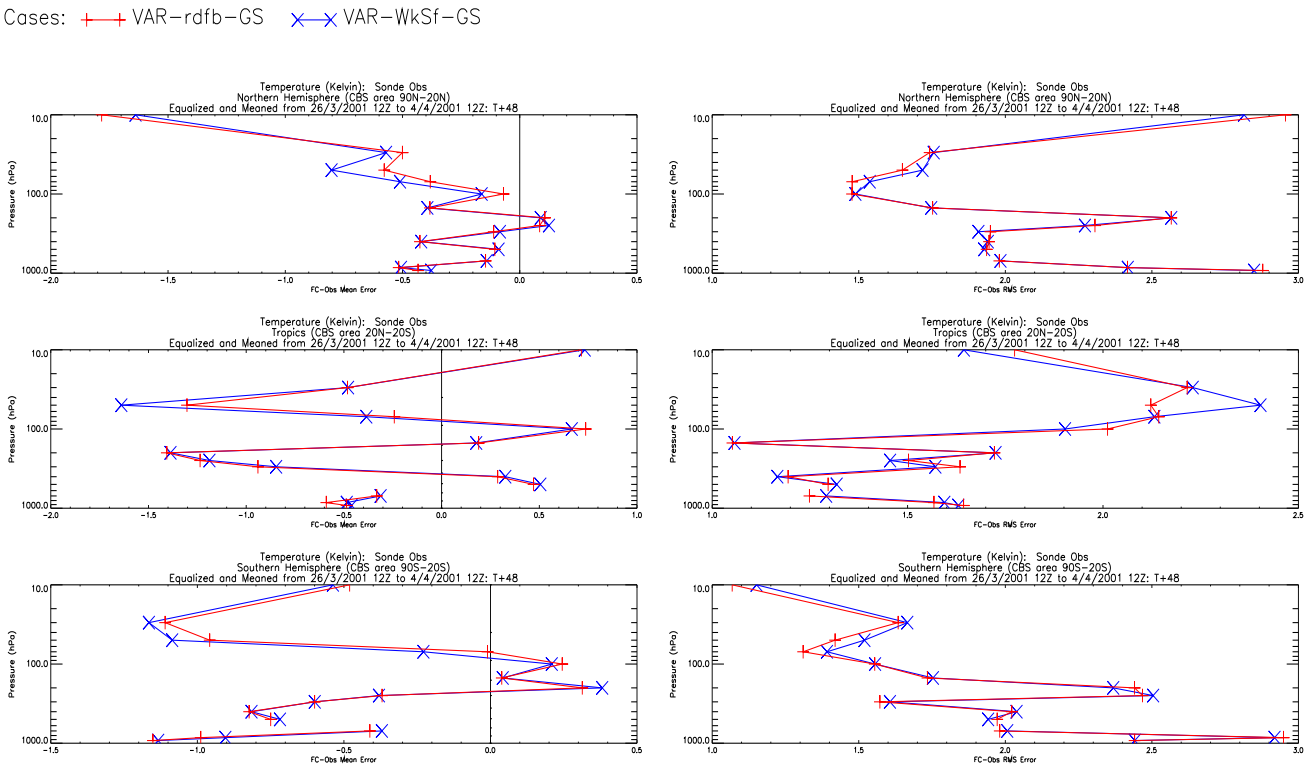

Figure 10: Mean and rms temperature errors, verified against sonde data, for 48 hour forecasts between 26/03/2001 and 04/04/2001. Two experiments are shown, without ozone-radiation interaction (blue line), with ozone-radiation interaction (red line). The errors are shown for three latitude zones: 20-90^{o}N, 20^{o}N-20^{o}S and 20-90^{o}S.

6 week-long forecast-only experiments were carried out to test the performance of these schemes. Results appear in Figure 12. The model field shown at the start of the run (21/09/2002) is the same as the climatological field for September taken from Li and Shine (1995), since that field is used to initialise the experiments. Multi-month ozone climatologies (eg Keating et al, 1996) show that the ozone field does not change greatly from one month to the next, so the initial field can act as a rough means of validating the ozone fields from later in the model runs. The field for 29/10/2002 from the run which uses the Cariolle parametrization is very similar to the initial field, with the major difference being that the ozone maximum in the tropics near 30 km is around 20 % greater. Therefore, this suggests that the Cariolle scheme is doing a reasonable job of parametrizing the chemistry needed to maintain the structure of the ozone field. By comparison, the ozone field for a run made without the Cariolle scheme appears poorer. The ozone maximum is smaller in both magnitude and area covered, ozone mixing ratios at levels above 40 km are 0.5-2.0 ppmv lower, and lower stratospheric mixing ratios are larger. These experiments were only run for 6 weeks, but multi-year runs made with the Old Dynamics model show that when the Cariolle scheme is not used the structure of the stratosphere ozone field is eventually eroded and the ozone becomes well mixed.

A further run was performed in which both Cariolle and cold tracer parametrizations were included. Figure 12 shows that the impact of the cold tracer scheme is to reduce ozone mixing ratios in the southern polar vortex, where temperatures are cold enough for PSCs to form.

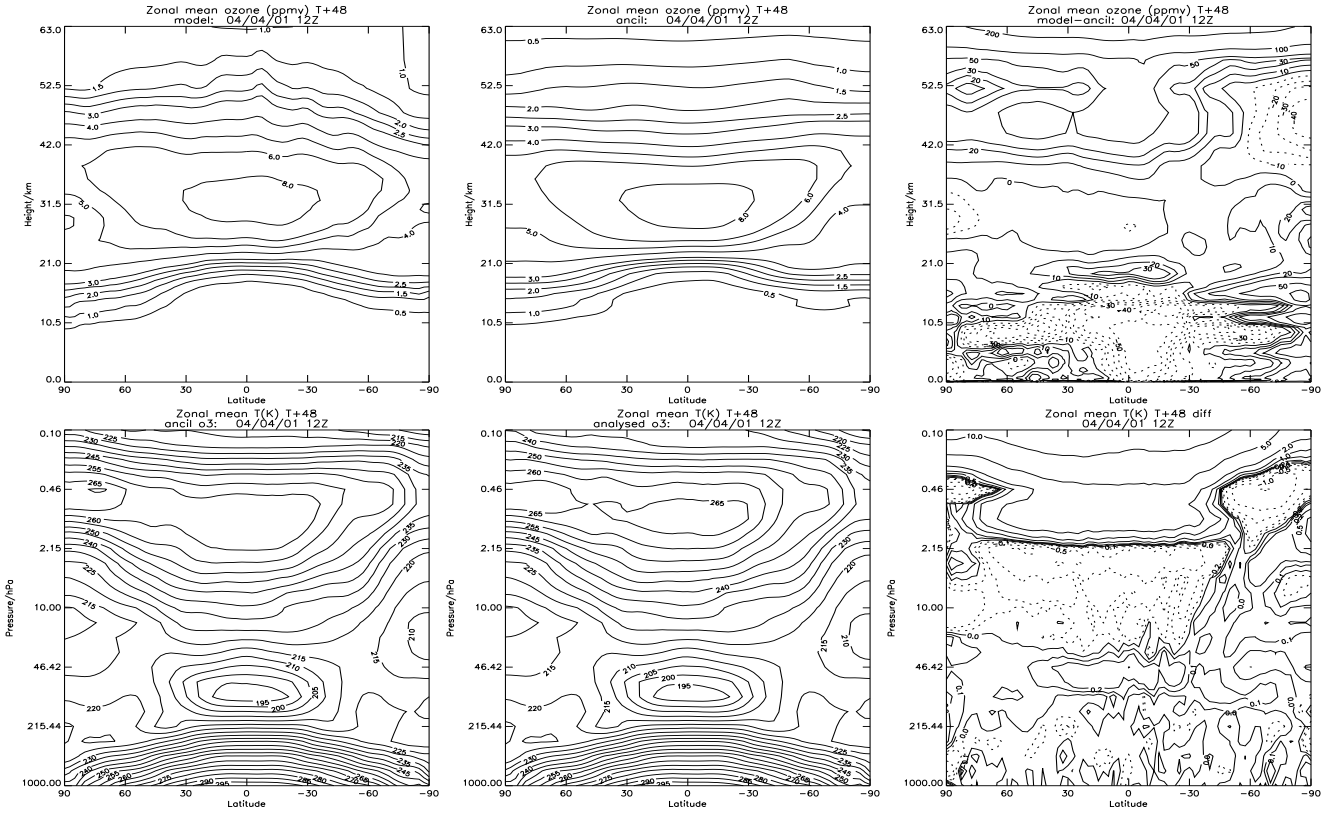

Figure 11: 48 hour ozone forecast field (run from 04/04/2001) for run with ozone-radiation interaction (upper left panel), corresponding field used in the model radiation scheme for the run without this interaction (which was derived from an ozone climatology) (upper centre panel), and the relative difference between these two fields (upper right panel). Units are ppmv for the first two fields are percentage for the last. Bottom panels show the 48 hour temperature forecast forecast field (run from 04/04/2001) for the runs with and without the ozone-radiation interaction (bottom left and bottom centre panels, respectively), and their difference (bottom right panels). Units are K. (NB: the vertical co-ordinate for the upper plots is height and for the lower plots is pressure. However, the range of the axes, and the tick marks shown, are approximately equivalent.)

These results indicate that both parametrizations perform adequately and that they can be used in ozone assimilation trials. Having said that, it was discovered that the Cariolle scheme is highly sensitive to variations in the overlying column abundance, and that it requires to be re-tuned each time the UM levels are changed (eg when switching from Old Dynamics to New Dynamics). It would make sense to test the performance of the Cariolle scheme further against other available schemes, such as the 'Linoz' scheme (McLinden et al, 2000) and the 'Chem2D' scheme (McCormack et al, 2004). A revised set of Cariolle scheme coefficients will shortly be received from Meteo-France and the performance of these will also be tested. A longer term approach may be to incorporate more sophisticated but highly computationally efficient ozone chemistry schemes which bear some similarities to the above schemes, but are non-linear and have a higher number of predictors. Such schemes have been successfully used in climate studies and are fast enough to be used for data assimilation (eg Taylor and Bourqui, pers. comm.)

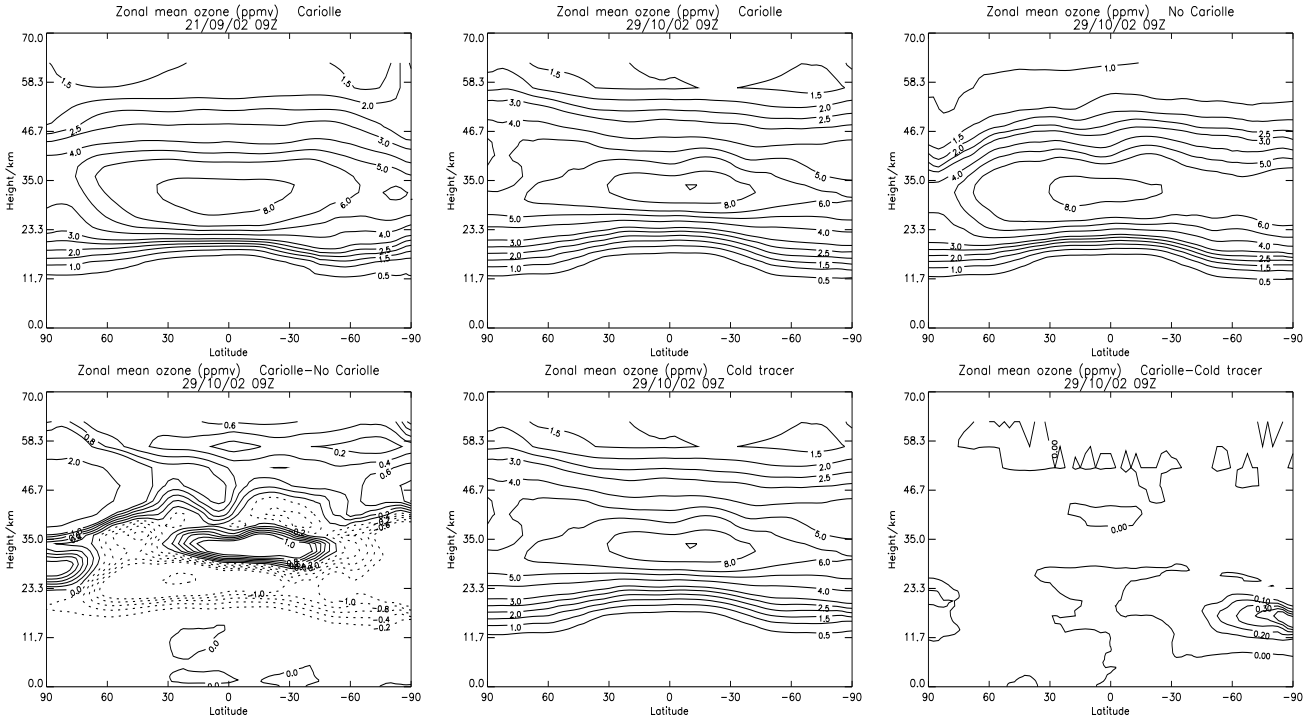

Figure 12: Model zonal mean ozone field for 21/09/02 (upper left panel) and 29/10/2002 (upper centre panel), for run with Cariolle scheme. Model zonal mean ozone field for 29/10/2002 for runs without Cariolle scheme (upper right panel) and with Cariolle and cold tracer schemes (lower centre panel), and differences between these fields and the field for the Cariolle only run (lower left and lower right panels, respectively). All fields are for 09Z. Units are ppmv.

5.1 Ozone Assimilation Trials with the Cariolle scheme

Two assimilation trials were carried out with the Cariolle scheme included: one where no ozone data is assimilated and one which assimilates ozone data from HIRS channel 9 and SBUV. These runs are then compared with similar trials in which the Cariolle scheme is not used (see Section 3). A further trial with the cold tracer parametrization included was run successfully for one day. This is important to note because, with Old Dynamics, it was impossible to get any assimilation trial to work using the cold tracer scheme. There was not enough time available, however, to complete the cold tracer trial and analyse the results. This should be done in the future.

First, the impact of the Cariolle scheme is investigated in trials where no ozone data are assimilated. In Figure 13 analysed total ozone is compared with GOME total ozone for two such trials. In general, the impact of the Cariolle is to cause a large reduction in the analysis error, most notably in the northern hemisphere and the tropics, where errors at the end of the run are around 25-35 DU smaller when the Cariolle is included that when it is not. In the southern hemisphere the corresponding improvement associated with the Cariolle scheme is 10-15 DU. A comparison of the results with ozonesonde profiles (Figure 14) shows that including the Cariolle scheme improves the quality of the background ozone at all levels between the troposphere and around 10 hPa. A further comparison with HALOE data (Figure 15) shows a similar pattern. However, above the mid stratosphere, the Cariolle scheme appears to over-estimate the ozone mixing ratio, and errors with

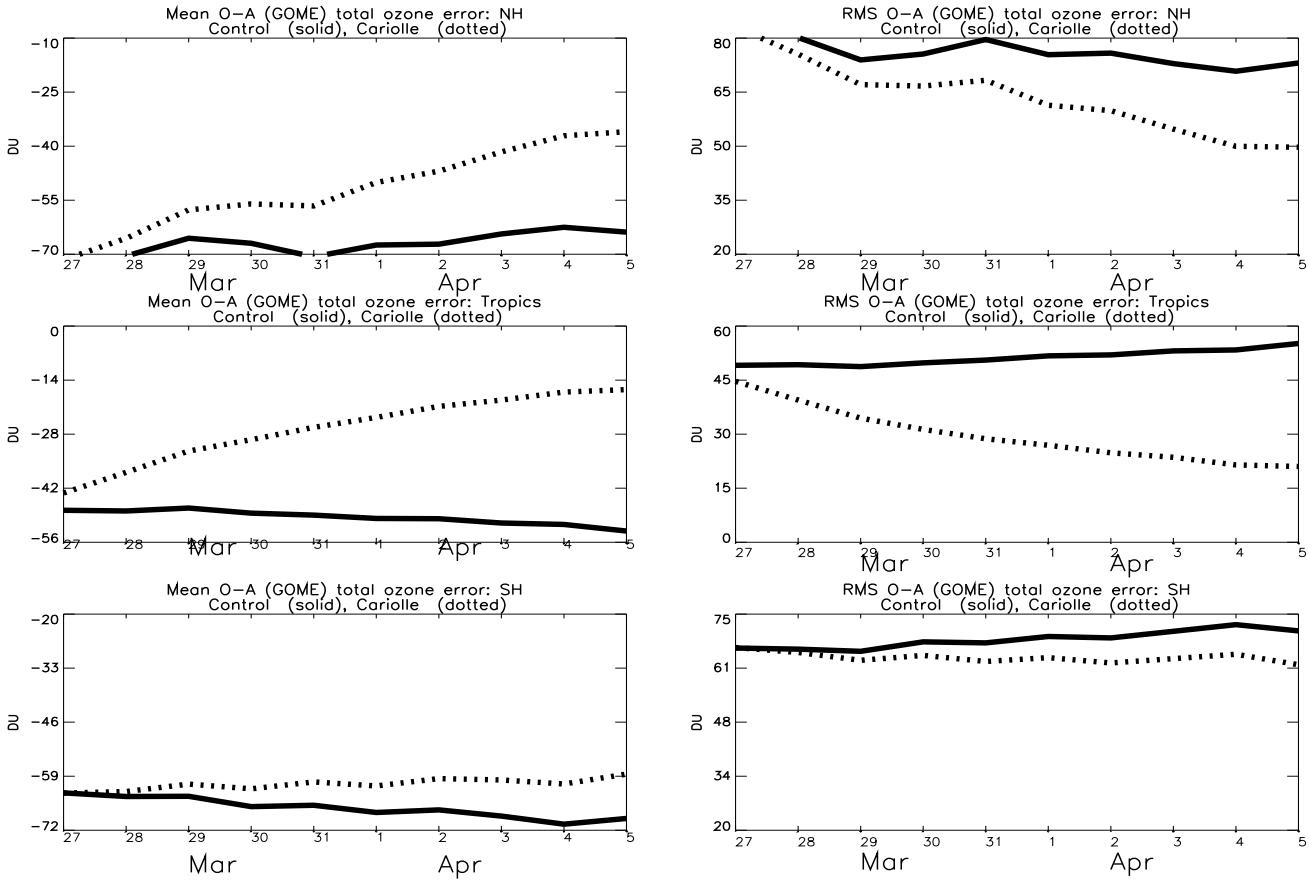

Figure 13: GOME total ozone minus analysed total ozone (DU), plotted against time, from 27/03/01-05/04/01. Mean (left panels) and RMS (right panels) for the northern hemisphere (30-90^{o}N) (top panels), tropics (30^{o}N-30^{o}S) (middle panels) and southern hemisphere (30-90^{o}S) (bottom panels). No ozone data are assimilated in the runs shown. Two runs are shown: Cariolle scheme not included (solid line), Cariolle scheme included (dotted line).

respect to the HALOE data are considerably greater than for the simulation where no Cariolle scheme is used. This may be because the Cariolle scheme has considerable sensitivity to changes in the overlying ozone column abundance, especially at upper levels.

It is striking that the impact of the Cariolle scheme on the total ozone error (Figure 13) is very similar to the impact of assimilating SBUV and HIRS channel 9 data (Figure 3). When these two changes are combined, will there be a further improvement in the ozone analyses, or is the effect of the assimilated ozone data only to correct large errors in the ozone background field which will be present when the Cariolle scheme is not used?

Figure 16 compares two assimilation trials which both include the Cariolle scheme. The first is a control run without ozone assimilation and the second is a run where SBUV and HIRS channel 9 data are assimilated. It can be seen that the impact of the assimilation is positive, though relatively small, less than 5 DU in the southern hemisphere and 5-15 DU elsewhere.

A comparison of ozone profiles for these trials with sonde data (Figure 17) shows that both sets of analyses are very similar. The clearest difference is in the northern hemisphere near 10 hPa, where results are better when no ozone data are assimilated. Close inspection also reveals a very slight improvement in the quality of the analyses in the upper troposphere and lower stratosphere when ozone data are added to the assimilation. Corresponding errors calculated with respect to HALOE data (not shown) generally confirm these results. They also show that the difference between the errors for both trials at levels above 10 hPa is

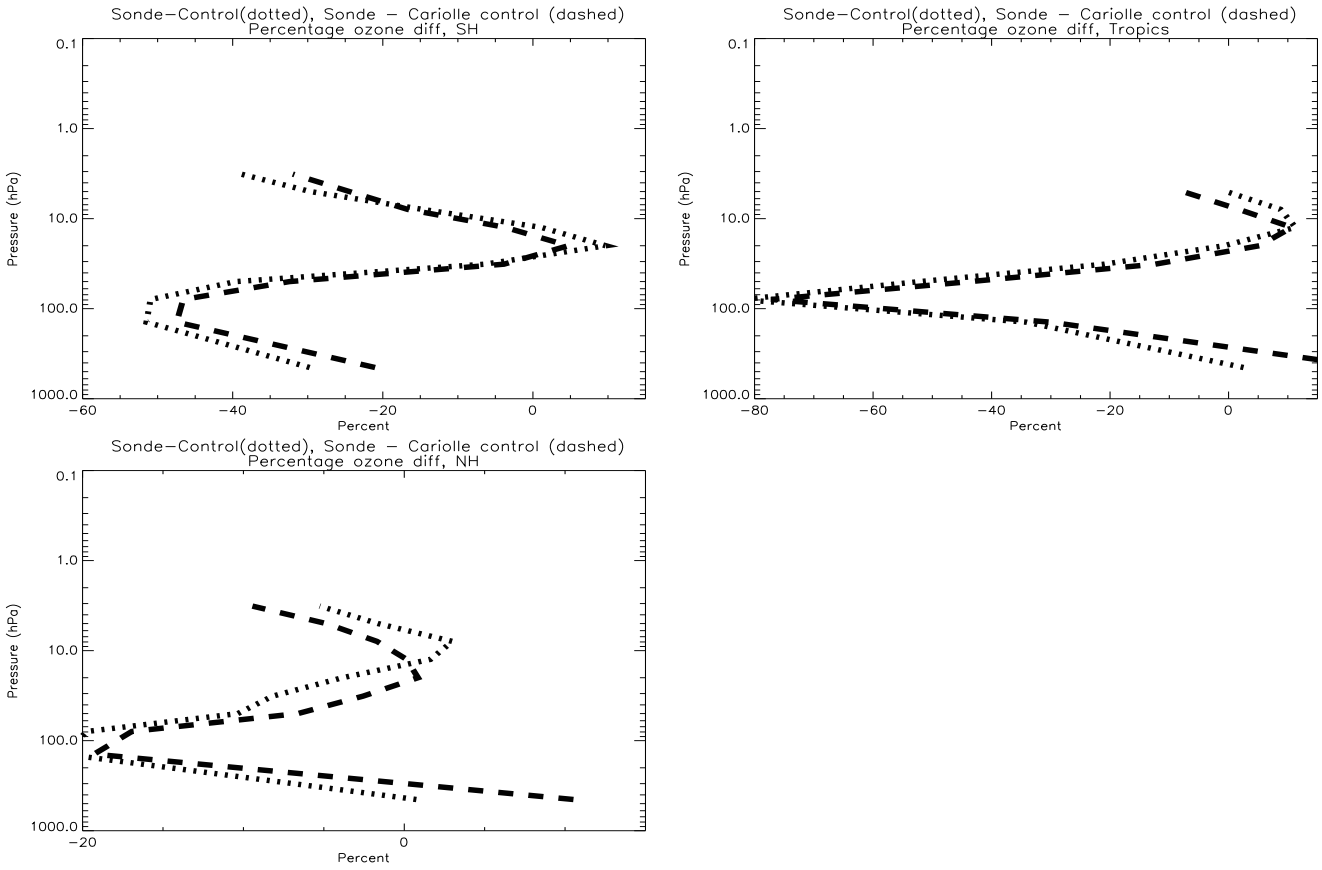

Figure 14: Percentage difference between ozonesonde and analysed ozone profiles (100 (O-A) / O, where O = sonde ozone and A=analysed ozone), averaged over the trial period (27/03/01-05/04/01). Profiles are shown for the southern hemisphere (30-90^{o}S), the the tropics (30^{o}N-30^{o}S) and the northern hemisphere (30-90^{o}N) for a run which excludes the Cariolle scheme (dotted line) and a run in which it is included (dashed line). In both runs, no ozone data is assimilated.

very small.

This result may indicate that further improvements to the ozone assimilation are required in order to better utilise the ozone data that are being assimilated. Such improvements may include improvements in the quality of the ozone background error covariances used. On the other hand, this may simply be an indication that the SBUV and HIRS channel 9 data are insufficient to properly describe the ozone field, since the SBUV observations are relatively sparse and are not available in the polar night, whilst the HIRS channel 9 data only provide information about the ozone field in the vicinity of the tropopause. Furthermore, the vertical resolution of these observations is low. These facts suggest that ozone data from other instruments need to be added to the assimilation system. Possible new instruments include the Advanced Infrared Sounder (AIRS), the Infrared Atmospheric Sounding Interferometer (IASI), the Global Ozone Monitoring Experiment 2 (GOME2), the High Resolution Dynamic Limb Sounder (HIRDLS) and data from the Envisat satellite, such as the Michaelson Interferometer for Passive Atmospheric Sounding (MIPAS). The latter dataset is already being assimilated, in collaboration with DARC, as part of the EU ASSET project.

6 Future Developments

In the near future, the following developments to the ozone assimilation system should be implemented.

1. *Extend existing tests*: As mentioned in Sections 4 and 5, the ozone-radiation interaction and chemistry parametrization tests should be extended to include longer-period assimilation trials, or

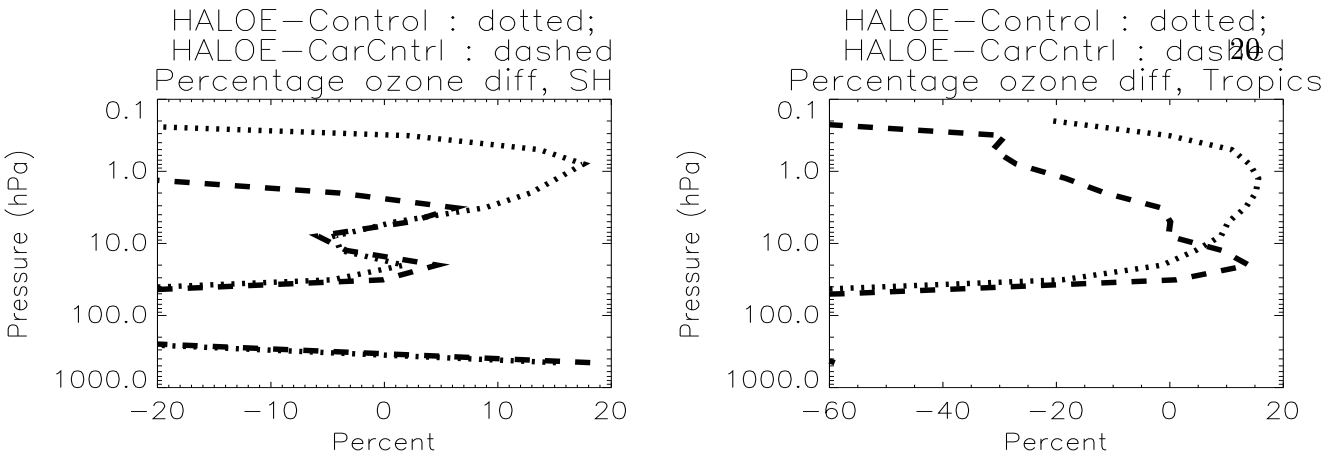

Figure 15: Percentage difference between HALOE and analysed ozone profiles (100 (O-A) / O, where O = HALOE ozone and A=analysed ozone), averaged over the trial period (27/03/01-05/04/01). The left panel shows values for the southern hemisphere (30-90^{o}S) and the right panel shows values for the tropics (30^{o}N-30^{o}S), for analyses run excluding Cariolle (dotted line) and including Cariolle (dashed line).

multi-annual climate simulations. As a general rule, the assimilation trial period should be extended from 10 days to one month and the trials run for different seasons.

2. *Improved ozone background error covariances*: Currently, the ozone background error covariances used are based on data supplied by ECMWF. However, these data describe errors in the ECMWF forecast model, which may be different from errors in the UM. In addition, these data may have been tuned to reduce analysis errors in the ECMWF system, but it does not follow that similar tuning is required for the Met Office ozone analysis. Thus, it is important that background errors be calculated from UM statistics, rather than imported from another model system. New approaches include recalculating ozone background error covariances using the NMC method (Parrish and Derber, 1992) or by using 6 hour differences from longer period runs (Y.J Rochon et al, pers. comm.).

3. *Extend system to include new observational data* Prime candidate is AIRS, which has recently been added to the operational NWP system. Other options include IASI, GOME 2, HIRDLS and MIPAS.

4. *Change the ozone background error covariances to include correlations with other analysis variables*: This may lead to improved analyses of both ozone and wind, particularly in the upper troposphere and lower stratosphere.

The benefits listed in 4) may be greater in 4D-Var than in 3D-Var. It is yet to be agreed whether ozone assimilation shall be added to the Met Office 4D-Var system, or whether future ozone developments shall be in line with the methodology (yet to be determined) which will be used in the Met Office Air Quality programme.

7 Summary

This paper has documented the processing and assimilation of layer mean ozone densities retrieved from SBUV data, and their implementation in the OPS and VAR code.

Initial trials with Old Dynamics and comparison with GOME data showed that including SBUV data often improved the ozone analyses, chiefly in the northern hemisphere where more SBUV data were available. Comparison with HALOE profiles showed a positive benefit from SBUV in the 50-5 hPa layer.

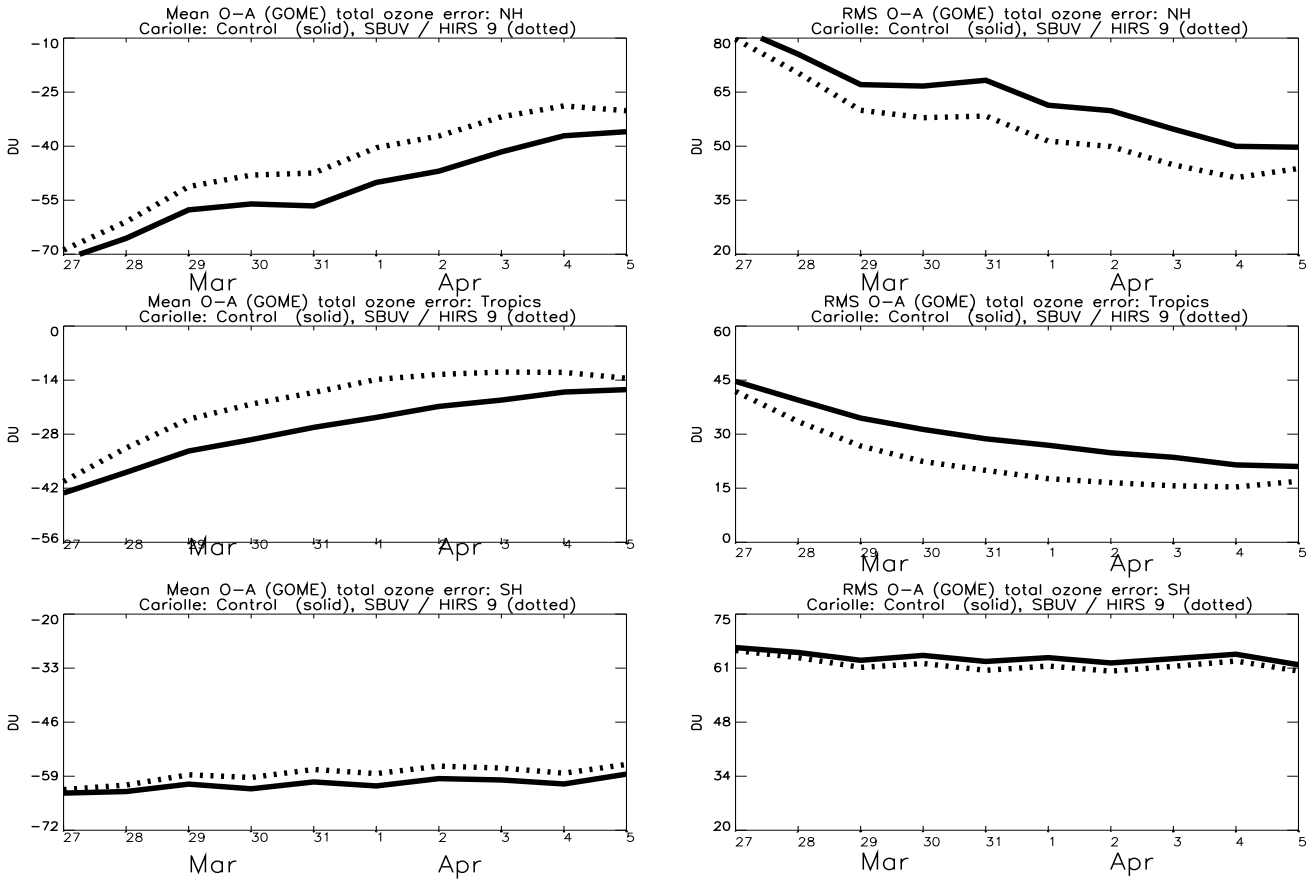

Figure 16: GOME total ozone minus analysed total ozone (DU), plotted against time, from 27/03/01-05/04/01. Mean (left panels) and RMS (right panels) for the northern hemisphere (30-90^{o}N) (top panels), tropics (30^{o}N-30^{o}S) (middle panels) and southern hemisphere (30-90^{o}S) (bottom panels). Two runs are shown: no ozone data assimilated (solid line), SBUV and HIRS channel 9 data assimilated (dotted line). Both runs include the Cariolle scheme.

The trials also showed that SBUV data did not improve the ozone analyses near the tropopause. There may be a case to omit SBUV data from the 1000-16 hPa layer from the assimilation, because of its poor vertical resolution. However, these results must be treated with some caution, because of the poor quality of the correlative HALOE data near the tropopause and the low numbers of SBUV observations available in the tropics and southern hemisphere during the trial period.

When the system was upgraded to run with New Dynamics an immediate difference was that the stratospheric peak in ozone in the start dump dropped in altitude. This was due to some feature of the Old Dynamics to New Dynamics reconfiguration. However, the reduction of errors compared to GOME occurred more rapidly with time for the New Dynamics trial than for the Old Dynamics trial, suggesting that the HIRS channel 9 and SBUV data were being properly assimilated and that the poor initial conditions gradually get spun out of the system.

A further upgrade to OPS Stable 20.1 revealed that more HIRS channel 9 were being rejected by the OPS than hitherto, and thus the impact of these data on the ozone analysis in the upper troposphere was reduced. It is not clear why this change in performance occurred, but a lot of the increased data rejections were due to the retrieved brightness temperatures failing their comparison against expected error. When the rejection limit for retrieved minus observed brightness temperature difference for HIRS channel 9 was increased by a factor of three, far more of these data were accepted by the OPS, and differences between analysed ozone and sonde data reduced, especially near the extratropical tropopause.

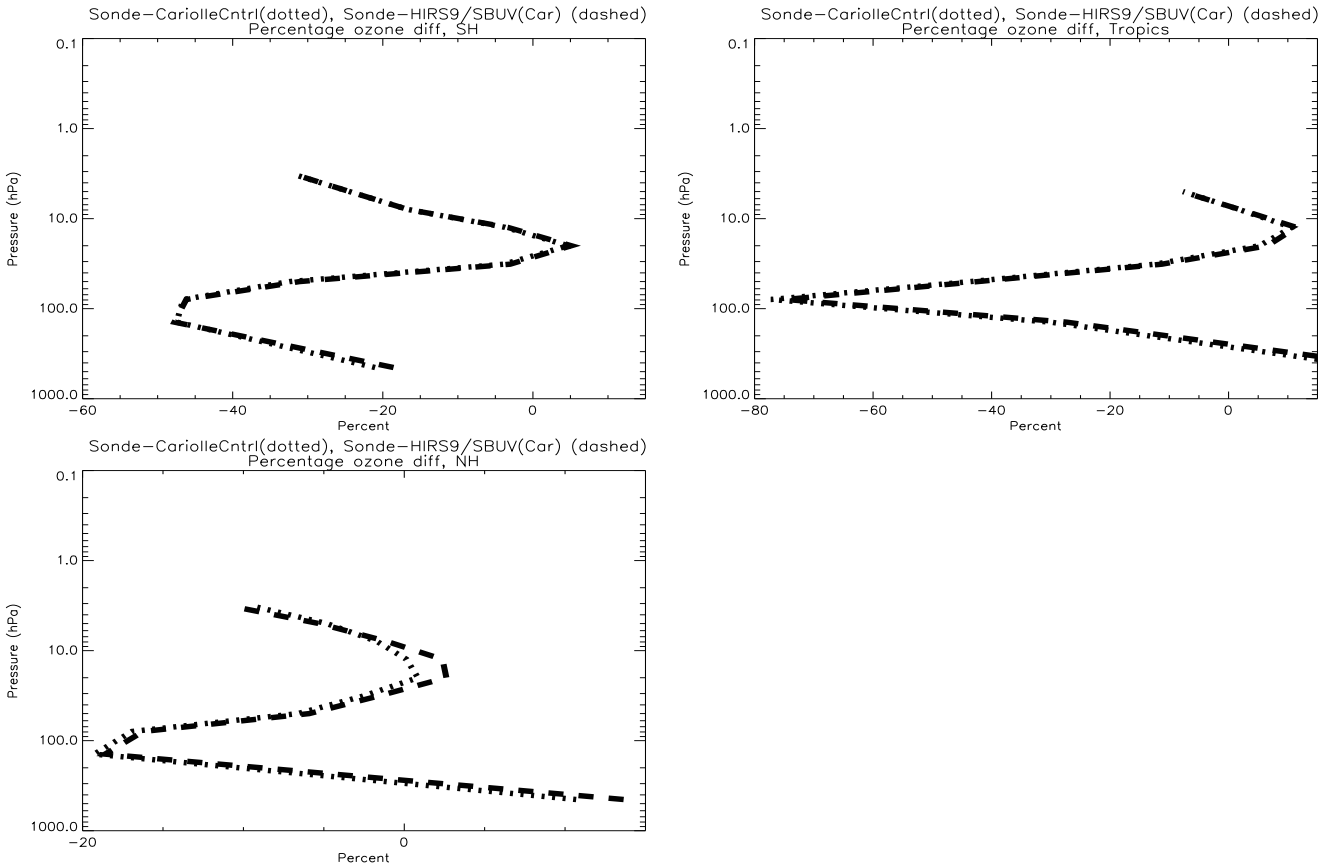

Figure 17: Percentage difference between ozonesonde and analysed ozone profiles (100 (O-A) / O, where O = sonde ozone and A=analysed ozone), averaged over the trial period (27/03/01-05/04/01). Profiles are shown for the southern hemisphere (30-90^{o}S), the the tropics (30^{o}N-30^{o}S) and the northern hemisphere (30-90^{o}N) for a run with no ozone assimilation (dotted line) and a run in which SBUV and HIRS channel 9 data are assimilated (dashed line). In both runs, the Cariolle scheme is switched on.

Allowing the analysed ozone to feed back to the model radiation scheme reduced temperature errors in the lower stratosphere. These results are encouraging and the experiments should be extended to include longer-period assimilation trials, or multi-annual climate simulations. A comparison of the results with a dataset of temperature correlative measurements in the mid and upper stratosphere is also required, since the impacts of the ozone-radiation interaction may be even larger at these levels.

The Cariolle and cold tracer ozone chemistry parametrization schemes were added to the UM and forecast-only trials suggested they were performing adequately. Inclusion of the Cariolle scheme in data assimilation trials had a large positive benefit in the ozone analysis. Furthermore, the relative benefit of assimilating SBUV and HIRS channel 9 data was smaller than in the trials where the Cariolle scheme was not used. This suggests that the ozone assimilation needs to be further improved, for example by improving the representation of background error covariances. However, it also may suggest that ozone data from SBUV and HIRS channel 9 are by themselves not sufficient to produce a large impact on the ozone analysis and that ozone data from other sources are required.

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